



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:40 AM UTC

PDB ID : 3DYM / pdb_00003dym
Title : E. coli (lacZ) beta-galactosidase (H418E)
Authors : Juers, D.H.; Huber, R.E.; Matthews, B.W.
Deposited on : 2008-07-28
Resolution : 2.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

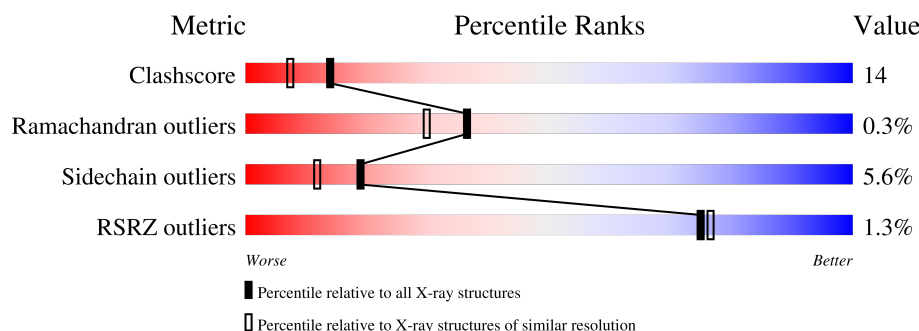
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1023	% 64% 28% 6% ..
1	B	1023	% 62% 30% 6% ..
1	C	1023	% 62% 29% 7% .
1	D	1023	% 64% 30% 5% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DMS	C	8504	-	-	X	-
4	DMS	D	8412	-	-	X	-
4	DMS	D	8419	-	-	X	-
4	DMS	D	8703	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36314 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	0	0	0
			8124	5137	1438	1511	38			
1	B	1011	Total	C	N	O	S	0	0	0
			8124	5137	1438	1511	38			
1	C	1011	Total	C	N	O	S	0	0	0
			8124	5137	1438	1511	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8124	5137	1438	1511	38			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P00722
A	2	SER	-	expression tag	UNP P00722
A	3	HIS	-	expression tag	UNP P00722
A	4	MET	-	expression tag	UNP P00722
A	5	LEU	-	expression tag	UNP P00722
A	6	GLU	-	expression tag	UNP P00722
A	7	ASP	-	expression tag	UNP P00722
A	8	PRO	-	expression tag	UNP P00722
A	418	GLU	HIS	engineered mutation	UNP P00722
B	1	GLY	-	expression tag	UNP P00722
B	2	SER	-	expression tag	UNP P00722
B	3	HIS	-	expression tag	UNP P00722
B	4	MET	-	expression tag	UNP P00722
B	5	LEU	-	expression tag	UNP P00722
B	6	GLU	-	expression tag	UNP P00722
B	7	ASP	-	expression tag	UNP P00722
B	8	PRO	-	expression tag	UNP P00722
B	418	GLU	HIS	engineered mutation	UNP P00722
C	1	GLY	-	expression tag	UNP P00722
C	2	SER	-	expression tag	UNP P00722
C	3	HIS	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	-	expression tag	UNP P00722
C	5	LEU	-	expression tag	UNP P00722
C	6	GLU	-	expression tag	UNP P00722
C	7	ASP	-	expression tag	UNP P00722
C	8	PRO	-	expression tag	UNP P00722
C	418	GLU	HIS	engineered mutation	UNP P00722
D	1	GLY	-	expression tag	UNP P00722
D	2	SER	-	expression tag	UNP P00722
D	3	HIS	-	expression tag	UNP P00722
D	4	MET	-	expression tag	UNP P00722
D	5	LEU	-	expression tag	UNP P00722
D	6	GLU	-	expression tag	UNP P00722
D	7	ASP	-	expression tag	UNP P00722
D	8	PRO	-	expression tag	UNP P00722
D	418	GLU	HIS	engineered mutation	UNP P00722

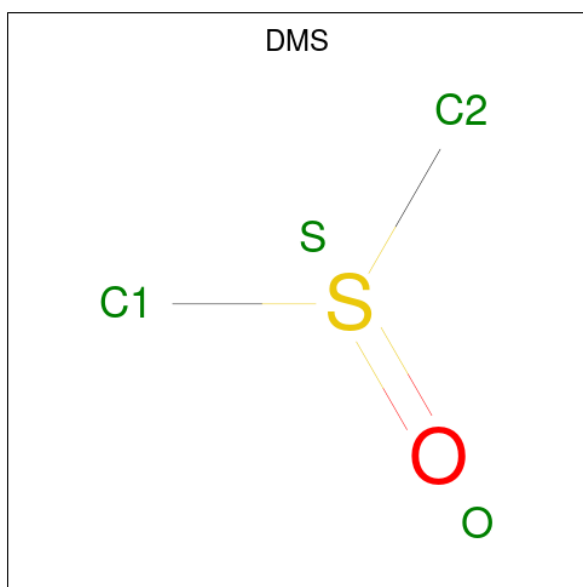
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Mg 4 4	0	0
2	B	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Na 4 4	0	0
3	B	4	Total Na 4 4	0	0
3	C	4	Total Na 4 4	0	0
3	D	4	Total Na 4 4	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0

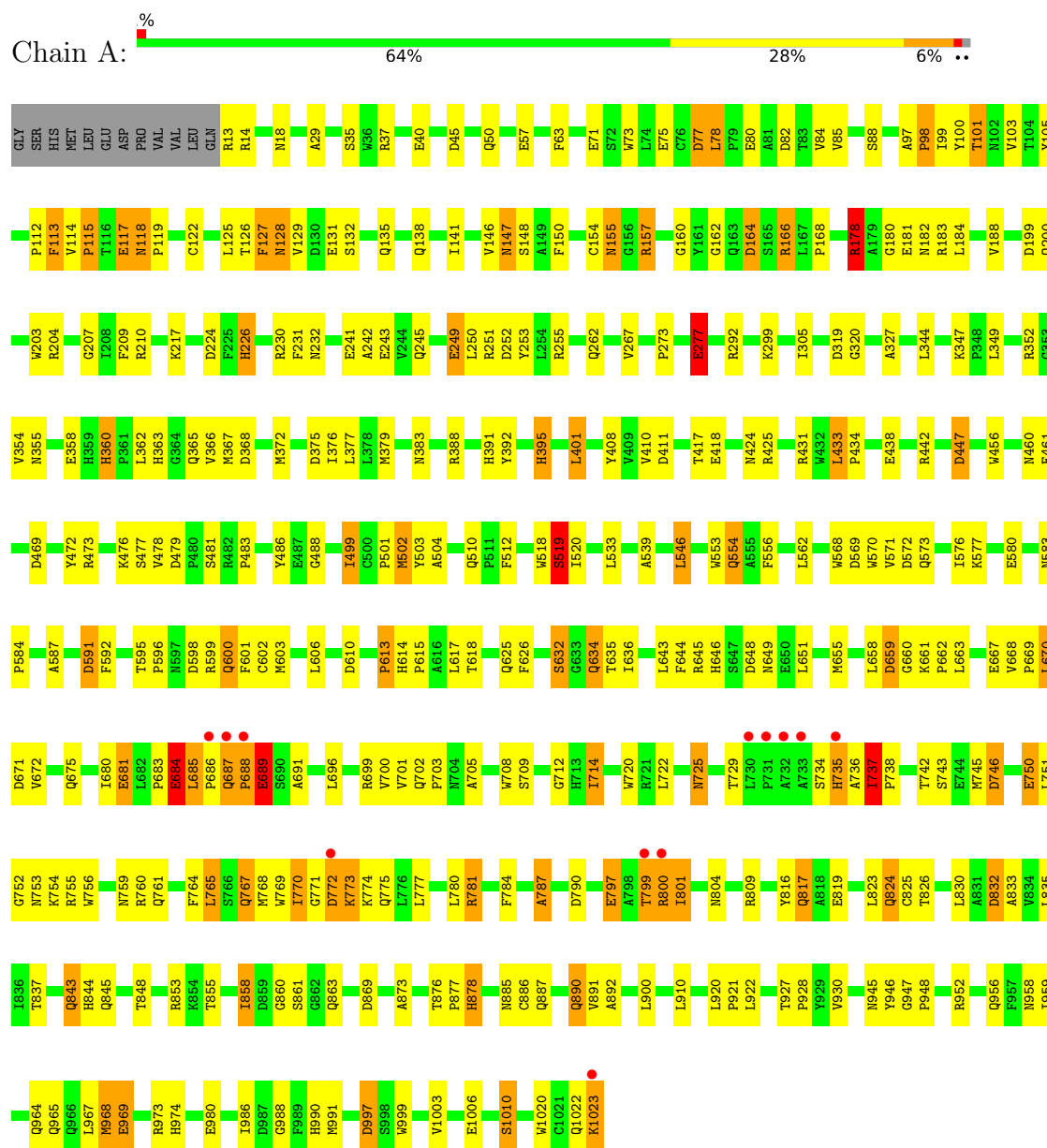
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	871	Total 871	O 871	0	0
5	B	864	Total 864	O 864	0	0
5	C	838	Total 838	O 838	0	0
5	D	891	Total 891	O 891	0	0

3 Residue-property plots

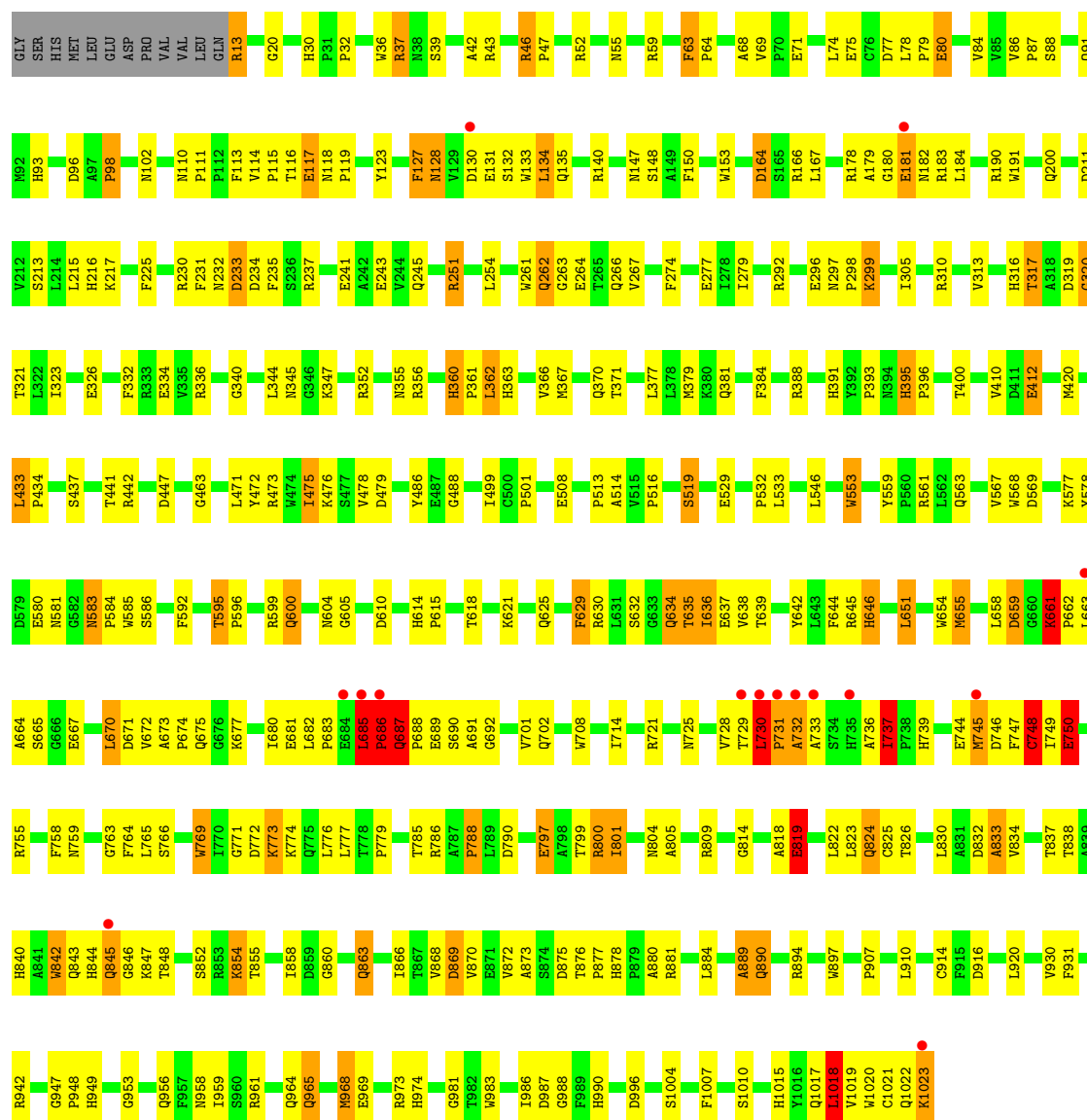
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Beta-galactosidase



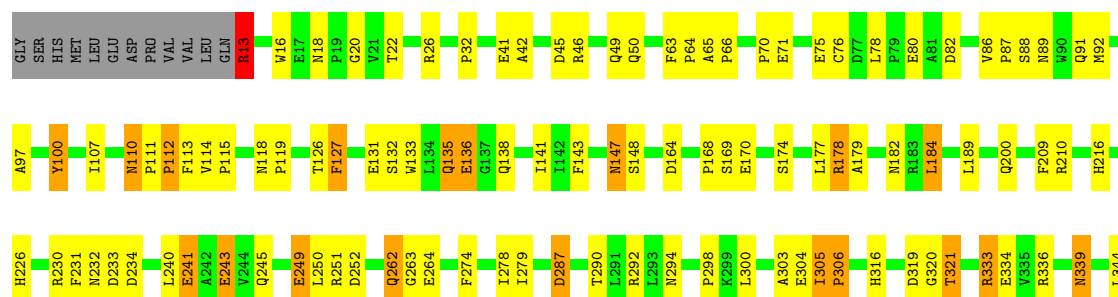
- Molecule 1: Beta-galactosidase

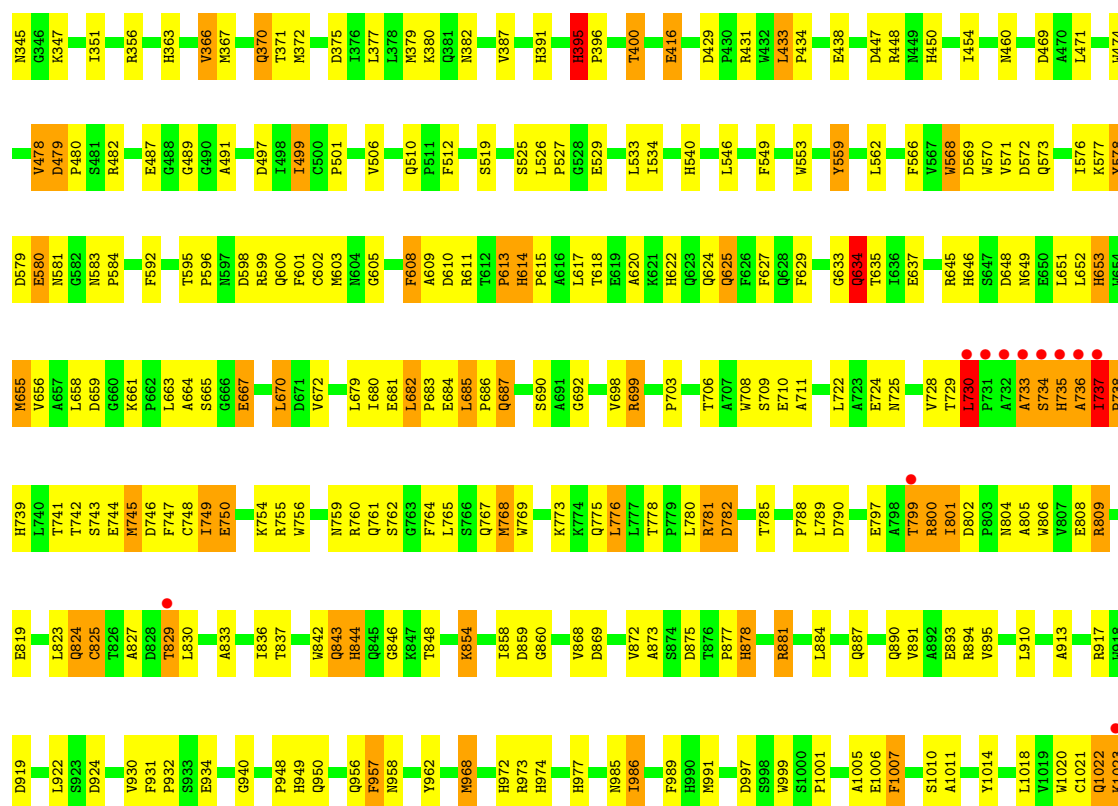
Chain B:  62% 30% 6% ..



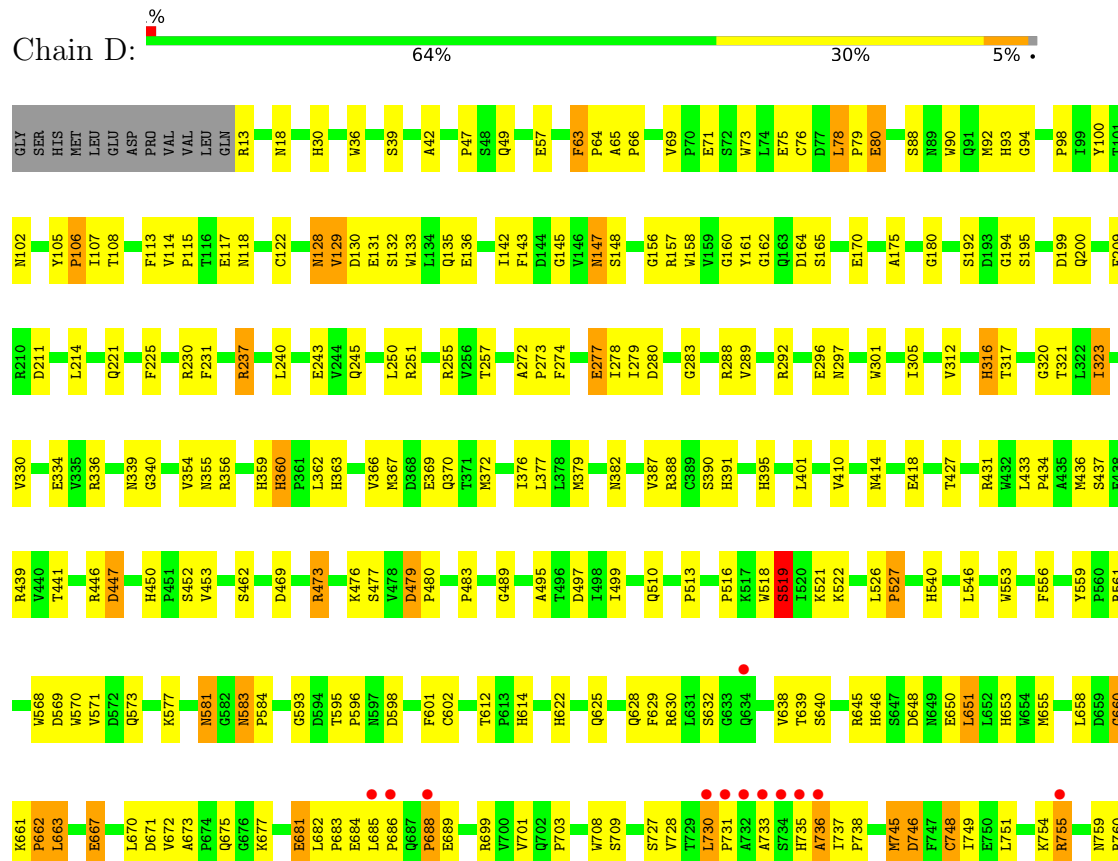
• Molecule 1: Beta-galactosidase

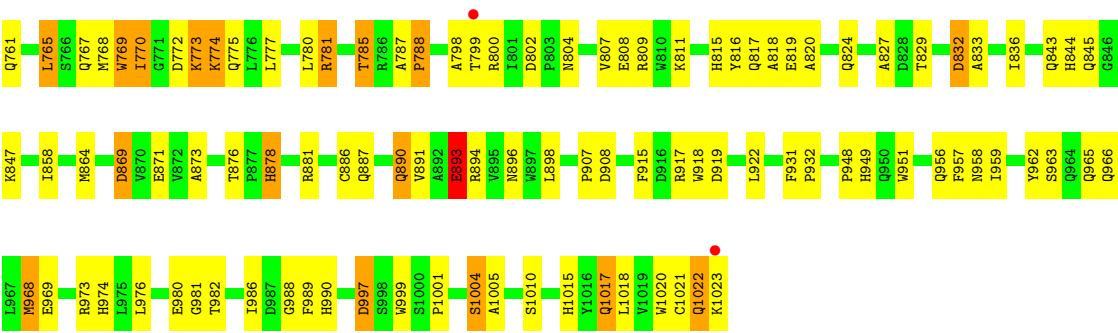
Chain C:  62% 29% 7% ..





● Molecule 1: Beta-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.34Å 167.16Å 200.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.50 – 2.05 34.50 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.50-2.05) 99.3 (34.50-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.05Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.158 , 0.251 0.158 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 109.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36314	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0670e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, DMS, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.25	9/8365 (0.1%)	1.89	175/11412 (1.5%)
1	B	1.25	0/8365	1.88	187/11412 (1.6%)
1	C	1.24	5/8365 (0.1%)	1.90	181/11412 (1.6%)
1	D	1.26	5/8365 (0.1%)	1.90	164/11412 (1.4%)
All	All	1.25	19/33460 (0.1%)	1.89	707/45648 (1.5%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	ASP	C-N	-7.99	1.25	1.34
1	C	479	ASP	C-N	-6.78	1.25	1.33
1	A	928	PRO	N-CA	-5.88	1.40	1.47
1	C	703	PRO	N-CA	-5.62	1.40	1.47
1	A	927	THR	C-O	-5.47	1.18	1.24

The worst 5 of 707 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	363	HIS	CA-CB-CG	-12.62	101.18	113.80
1	A	790	ASP	CA-CB-CG	-11.60	101.00	112.60
1	B	363	HIS	CA-CB-CG	-10.99	102.81	113.80
1	A	583	ASN	CA-CB-CG	-10.58	102.02	112.60
1	B	737	ILE	N-CA-CB	10.28	122.61	111.61

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8124	0	7715	212	0
1	B	8124	0	7715	245	0
1	C	8124	0	7715	251	0
1	D	8124	0	7715	206	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	68	0	102	15	0
4	B	76	0	114	17	0
4	C	92	0	138	21	0
4	D	92	0	138	25	0
5	A	871	0	0	19	0
5	B	864	0	0	20	0
5	C	838	0	0	17	0
5	D	891	0	0	24	0
All	All	36314	0	31352	921	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 921 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.32	1.26
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.42	1.18
1:C:634:GLN:H	1:C:634:GLN:NE2	1.46	1.11
1:B:744:GLU:HB2	1:B:745:MET:HE3	1.21	1.11
1:C:765:LEU:HD21	1:C:768:MET:HE2	1.33	1.09

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1009/1023 (99%)	963 (95%)	44 (4%)	2 (0%)	43	37
1	B	1009/1023 (99%)	965 (96%)	36 (4%)	8 (1%)	16	9
1	C	1009/1023 (99%)	961 (95%)	47 (5%)	1 (0%)	48	43
1	D	1009/1023 (99%)	958 (95%)	48 (5%)	3 (0%)	36	30
All	All	4036/4092 (99%)	3847 (95%)	175 (4%)	14 (0%)	36	30

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	688	PRO
1	B	690	SER
1	B	731	PRO
1	A	689	GLU
1	D	688	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	864/875 (99%)	823 (95%)	41 (5%)	23	17
1	B	864/875 (99%)	809 (94%)	55 (6%)	16	9
1	C	864/875 (99%)	812 (94%)	52 (6%)	17	10
1	D	864/875 (99%)	817 (95%)	47 (5%)	20	12
All	All	3456/3500 (99%)	3261 (94%)	195 (6%)	19	12

5 of 195 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	580	GLU
1	C	956	GLN
1	C	663	LEU
1	C	749	ILE
1	D	71	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	266	GLN
1	D	485	GLN
1	D	878	HIS
1	B	653	HIS
1	B	646	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 108 ligands modelled in this entry, 26 are monoatomic - leaving 82 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	C	8401	-	3,3,3	1.63	1 (33%)	3,3,3	0.29	0
4	DMS	C	8425	3	3,3,3	1.53	1 (33%)	3,3,3	0.33	0
4	DMS	C	8419	-	3,3,3	0.80	0	3,3,3	0.31	0
4	DMS	C	8402	-	3,3,3	1.42	1 (33%)	3,3,3	0.09	0
4	DMS	D	8402	-	3,3,3	0.63	0	3,3,3	0.48	0
4	DMS	D	8508	-	3,3,3	1.04	0	3,3,3	0.27	0
4	DMS	C	8420	-	3,3,3	1.74	1 (33%)	3,3,3	0.07	0
4	DMS	C	8501	-	3,3,3	1.39	0	3,3,3	0.47	0
4	DMS	D	8420	-	3,3,3	1.60	1 (33%)	3,3,3	0.27	0
4	DMS	C	8506	-	3,3,3	1.65	1 (33%)	3,3,3	0.25	0
4	DMS	B	8416	-	3,3,3	0.85	0	3,3,3	0.36	0
4	DMS	D	8703	-	3,3,3	0.75	0	3,3,3	0.48	0
4	DMS	D	8421	-	3,3,3	0.55	0	3,3,3	0.12	0
4	DMS	B	8411	-	3,3,3	1.22	1 (33%)	3,3,3	0.23	0
4	DMS	A	8404	-	3,3,3	1.24	0	3,3,3	0.46	0
4	DMS	D	8501	-	3,3,3	0.53	0	3,3,3	0.35	0
4	DMS	B	8421	-	3,3,3	0.71	0	3,3,3	0.59	0
4	DMS	B	8409	-	3,3,3	1.71	1 (33%)	3,3,3	0.38	0
4	DMS	D	8401	-	3,3,3	1.39	1 (33%)	3,3,3	0.85	0
4	DMS	C	8404	-	3,3,3	1.50	1 (33%)	3,3,3	1.18	1 (33%)
4	DMS	D	8425	3	3,3,3	0.45	0	3,3,3	0.34	0
4	DMS	B	8402	-	3,3,3	0.80	0	3,3,3	0.53	0
4	DMS	D	8419	-	3,3,3	1.37	1 (33%)	3,3,3	0.91	0
4	DMS	A	8411	-	3,3,3	0.70	0	3,3,3	0.10	0
4	DMS	B	8508	-	3,3,3	1.68	1 (33%)	3,3,3	0.91	0
4	DMS	C	8421	-	3,3,3	0.52	0	3,3,3	0.19	0
4	DMS	D	8404	-	3,3,3	1.19	0	3,3,3	0.16	0
4	DMS	D	8408	-	3,3,3	0.57	0	3,3,3	0.32	0
4	DMS	D	8405	-	3,3,3	1.17	0	3,3,3	1.12	0
4	DMS	B	8408	-	3,3,3	0.77	0	3,3,3	1.40	1 (33%)
4	DMS	A	8405	-	3,3,3	1.62	1 (33%)	3,3,3	0.22	0
4	DMS	B	8504	-	3,3,3	0.98	0	3,3,3	0.64	0
4	DMS	C	8602	-	3,3,3	1.69	1 (33%)	3,3,3	0.23	0
4	DMS	A	8403	-	3,3,3	2.05	2 (66%)	3,3,3	0.72	0
4	DMS	D	8412	-	3,3,3	0.89	0	3,3,3	0.40	0
4	DMS	A	8409	-	3,3,3	1.60	1 (33%)	3,3,3	0.19	0
4	DMS	D	8705	-	3,3,3	0.28	0	3,3,3	1.08	0
4	DMS	C	8416	-	3,3,3	0.77	0	3,3,3	0.44	0
4	DMS	B	8403	-	3,3,3	1.78	1 (33%)	3,3,3	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	D	8411	-	3,3,3	0.87	0	3,3,3	0.13	0
4	DMS	B	8414	-	3,3,3	0.72	0	3,3,3	0.46	0
4	DMS	A	8416	-	3,3,3	1.07	0	3,3,3	0.50	0
4	DMS	A	8602	-	3,3,3	1.18	0	3,3,3	0.20	0
4	DMS	A	8414	-	3,3,3	0.83	0	3,3,3	0.19	0
4	DMS	C	8411	-	3,3,3	1.22	0	3,3,3	0.38	0
4	DMS	A	8412	-	3,3,3	0.88	0	3,3,3	0.46	0
4	DMS	B	8412	-	3,3,3	1.22	0	3,3,3	0.25	0
4	DMS	C	8423	-	3,3,3	0.55	0	3,3,3	0.45	0
4	DMS	C	8409	-	3,3,3	0.93	0	3,3,3	0.27	0
4	DMS	D	8409	-	3,3,3	1.27	1 (33%)	3,3,3	0.39	0
4	DMS	A	8425	3	3,3,3	1.08	0	3,3,3	0.19	0
4	DMS	B	8601	-	3,3,3	1.20	0	3,3,3	0.45	0
4	DMS	B	8423	-	3,3,3	0.89	0	3,3,3	0.55	0
4	DMS	C	8414	-	3,3,3	0.95	0	3,3,3	0.24	0
4	DMS	B	8417	-	3,3,3	0.46	0	3,3,3	0.27	0
4	DMS	A	8421	-	3,3,3	1.11	0	3,3,3	0.23	0
4	DMS	C	8601	-	3,3,3	1.93	1 (33%)	3,3,3	0.64	0
4	DMS	C	8417	-	3,3,3	0.11	0	3,3,3	0.50	0
4	DMS	B	8425	3	3,3,3	1.71	1 (33%)	3,3,3	0.20	0
4	DMS	A	8501	-	3,3,3	1.46	0	3,3,3	0.52	0
4	DMS	A	8504	-	3,3,3	0.48	0	3,3,3	0.33	0
4	DMS	D	8701	-	3,3,3	1.77	1 (33%)	3,3,3	1.00	0
4	DMS	A	8402	-	3,3,3	1.34	0	3,3,3	0.33	0
4	DMS	D	8406	-	3,3,3	1.14	0	3,3,3	0.65	0
4	DMS	C	8504	-	3,3,3	0.45	0	3,3,3	0.29	0
4	DMS	D	8414	-	3,3,3	0.42	0	3,3,3	0.08	0
4	DMS	C	8408	-	3,3,3	1.17	0	3,3,3	0.54	0
4	DMS	B	8404	-	3,3,3	0.36	0	3,3,3	0.66	0
4	DMS	D	8416	-	3,3,3	1.22	1 (33%)	3,3,3	0.23	0
4	DMS	A	8401	-	3,3,3	0.56	0	3,3,3	0.34	0
4	DMS	D	8506	-	3,3,3	1.96	1 (33%)	3,3,3	0.44	0
4	DMS	C	8403	-	3,3,3	1.61	1 (33%)	3,3,3	0.26	0
4	DMS	D	8403	-	3,3,3	2.03	1 (33%)	3,3,3	0.36	0
4	DMS	C	8407	-	3,3,3	2.22	2 (66%)	3,3,3	0.21	0
4	DMS	B	8406	-	3,3,3	0.67	0	3,3,3	0.27	0
4	DMS	C	8412	-	3,3,3	0.55	0	3,3,3	0.45	0
4	DMS	B	8401	-	3,3,3	1.12	0	3,3,3	0.56	0
4	DMS	C	8405	-	3,3,3	1.72	1 (33%)	3,3,3	0.30	0
4	DMS	A	8408	-	3,3,3	0.36	0	3,3,3	0.10	0
4	DMS	A	8406	-	3,3,3	0.78	0	3,3,3	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	B	8405	-	3,3,3	1.76	1 (33%)	3,3,3	0.34	0
4	DMS	D	8423	-	3,3,3	1.15	0	3,3,3	0.27	0

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	8506	DMS	O-S	3.26	1.71	1.50
4	C	8601	DMS	C2-S	3.25	1.99	1.76
4	B	8405	DMS	O-S	2.94	1.69	1.50
4	D	8403	DMS	C2-S	2.87	1.96	1.76
4	B	8409	DMS	O-S	2.85	1.69	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	8408	DMS	C2-S-C1	2.42	110.81	98.42
4	C	8404	DMS	C2-S-C1	2.02	108.77	98.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

38 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	8425	DMS	2	0
4	C	8419	DMS	2	0
4	C	8402	DMS	1	0
4	C	8420	DMS	2	0
4	C	8501	DMS	1	0
4	B	8416	DMS	3	0
4	D	8703	DMS	5	0
4	A	8404	DMS	1	0
4	C	8404	DMS	1	0
4	D	8425	DMS	1	0
4	D	8419	DMS	8	0
4	D	8404	DMS	2	0
4	B	8408	DMS	1	0
4	B	8504	DMS	3	0
4	A	8403	DMS	1	0
4	D	8412	DMS	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	8416	DMS	1	0
4	B	8403	DMS	1	0
4	D	8411	DMS	1	0
4	A	8416	DMS	3	0
4	A	8602	DMS	1	0
4	A	8414	DMS	1	0
4	A	8412	DMS	3	0
4	C	8423	DMS	1	0
4	A	8425	DMS	2	0
4	B	8601	DMS	1	0
4	B	8423	DMS	1	0
4	B	8417	DMS	2	0
4	C	8417	DMS	2	0
4	A	8501	DMS	2	0
4	C	8504	DMS	4	0
4	B	8404	DMS	2	0
4	D	8506	DMS	2	0
4	C	8403	DMS	3	0
4	B	8406	DMS	3	0
4	C	8412	DMS	1	0
4	A	8406	DMS	1	0
4	D	8423	DMS	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1011/1023 (98%)	-0.60	12 (1%) 76 78	9, 22, 53, 100	0
1	B	1011/1023 (98%)	-0.50	15 (1%) 72 73	11, 23, 54, 100	0
1	C	1011/1023 (98%)	-0.53	11 (1%) 78 80	10, 23, 55, 99	0
1	D	1011/1023 (98%)	-0.57	14 (1%) 73 75	10, 23, 53, 100	0
All	All	4044/4092 (98%)	-0.55	52 (1%) 75 76	9, 23, 54, 100	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	685	LEU	4.3
1	A	686	PRO	4.3
1	D	734	SER	4.1
1	C	736	ALA	3.9
1	B	745	MET	3.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DMS	A	8416	4/4	0.79	0.20	36,66,91,100	0
4	DMS	B	8406	4/4	0.85	0.22	38,56,100,100	0
4	DMS	C	8506	4/4	0.85	0.19	51,54,73,100	0
4	DMS	C	8407	4/4	0.86	0.19	24,32,100,100	0
4	DMS	A	8421	4/4	0.86	0.19	68,73,83,100	0
4	DMS	B	8508	4/4	0.87	0.17	46,49,56,100	0
2	MG	A	3005	1/1	0.88	0.10	44,44,44,44	0
4	DMS	A	8406	4/4	0.88	0.13	26,35,53,78	0
4	DMS	D	8420	4/4	0.88	0.21	39,58,78,100	0
4	DMS	D	8416	4/4	0.88	0.16	49,54,72,100	0
4	DMS	D	8703	4/4	0.88	0.20	31,67,78,79	0
4	DMS	C	8416	4/4	0.89	0.16	65,77,100,100	0
4	DMS	C	8421	4/4	0.89	0.17	52,71,78,100	0
4	DMS	D	8421	4/4	0.89	0.17	51,71,100,100	0
4	DMS	B	8417	4/4	0.89	0.13	27,30,49,75	0
4	DMS	A	8501	4/4	0.90	0.10	28,32,54,59	0
4	DMS	B	8414	4/4	0.91	0.15	26,59,70,100	0
4	DMS	B	8416	4/4	0.91	0.11	37,39,76,100	0
4	DMS	A	8414	4/4	0.91	0.16	49,55,92,97	0
4	DMS	C	8417	4/4	0.91	0.12	24,40,50,61	0
4	DMS	D	8423	4/4	0.91	0.18	36,56,77,100	0
4	DMS	B	8423	4/4	0.91	0.16	53,53,74,80	0
4	DMS	B	8421	4/4	0.92	0.12	34,52,77,100	0
4	DMS	D	8414	4/4	0.92	0.16	43,63,100,100	0
4	DMS	A	8602	4/4	0.92	0.21	57,95,100,100	0
3	NA	D	3104	1/1	0.92	0.08	44,44,44,44	0
4	DMS	B	8408	4/4	0.92	0.15	29,44,44,67	0
4	DMS	D	8506	4/4	0.92	0.17	60,82,100,100	0
4	DMS	C	8601	4/4	0.92	0.12	33,41,60,73	0
4	DMS	D	8705	4/4	0.92	0.11	36,42,50,52	0
3	NA	B	3104	1/1	0.93	0.08	39,39,39,39	0
4	DMS	C	8504	4/4	0.93	0.16	43,75,100,100	0
4	DMS	A	8504	4/4	0.93	0.19	27,49,100,100	0
4	DMS	C	8420	4/4	0.93	0.16	42,62,86,100	0
4	DMS	D	8409	4/4	0.94	0.11	41,44,46,57	0
4	DMS	B	8504	4/4	0.94	0.11	36,38,60,100	0
4	DMS	B	8404	4/4	0.94	0.09	29,30,56,60	0
4	DMS	D	8419	4/4	0.94	0.12	47,59,83,92	0
4	DMS	C	8423	4/4	0.94	0.12	53,55,57,75	0
4	DMS	A	8411	4/4	0.94	0.14	30,45,54,100	0
3	NA	C	3104	1/1	0.94	0.07	36,36,36,36	0
4	DMS	D	8508	4/4	0.94	0.13	41,50,71,78	0
4	DMS	A	8425	4/4	0.94	0.12	37,39,60,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DMS	C	8419	4/4	0.94	0.16	61,79,85,100	0
4	DMS	C	8409	4/4	0.95	0.10	46,50,57,63	0
4	DMS	C	8414	4/4	0.95	0.16	26,46,100,100	0
4	DMS	C	8425	4/4	0.95	0.16	37,50,100,100	0
3	NA	D	3103	1/1	0.95	0.05	35,35,35,35	0
2	MG	A	3105	1/1	0.95	0.05	32,32,32,32	0
4	DMS	A	8412	4/4	0.95	0.11	39,39,50,100	0
4	DMS	C	8602	4/4	0.95	0.16	22,65,100,100	0
4	DMS	C	8408	4/4	0.95	0.10	23,41,44,44	0
4	DMS	D	8403	4/4	0.95	0.11	31,32,49,67	0
4	DMS	D	8404	4/4	0.95	0.13	22,40,56,100	0
4	DMS	A	8409	4/4	0.96	0.10	39,42,46,48	0
4	DMS	B	8409	4/4	0.96	0.08	33,37,37,47	0
4	DMS	C	8412	4/4	0.96	0.17	39,43,96,100	0
4	DMS	B	8425	4/4	0.96	0.07	30,33,44,55	0
3	NA	A	3104	1/1	0.96	0.04	32,32,32,32	0
4	DMS	A	8404	4/4	0.96	0.10	25,37,51,61	0
4	DMS	D	8425	4/4	0.96	0.14	13,26,31,59	4
4	DMS	D	8501	4/4	0.96	0.10	42,42,53,66	0
4	DMS	B	8601	4/4	0.96	0.12	44,57,68,100	0
4	DMS	C	8403	4/4	0.96	0.08	23,30,41,44	0
3	NA	C	3103	1/1	0.96	0.06	37,37,37,37	0
4	DMS	D	8406	4/4	0.96	0.10	24,25,33,49	0
4	DMS	A	8408	4/4	0.97	0.10	32,37,50,100	0
2	MG	D	3001	1/1	0.97	0.03	26,26,26,26	0
4	DMS	C	8501	4/4	0.97	0.07	25,30,42,49	0
4	DMS	C	8411	4/4	0.97	0.09	38,38,50,72	0
4	DMS	A	8405	4/4	0.97	0.08	28,38,39,40	0
4	DMS	B	8411	4/4	0.97	0.10	22,42,43,100	0
4	DMS	B	8412	4/4	0.97	0.11	32,46,48,78	0
4	DMS	B	8403	4/4	0.97	0.08	33,35,41,47	0
4	DMS	A	8403	4/4	0.97	0.11	32,36,46,67	0
4	DMS	C	8404	4/4	0.97	0.07	18,24,38,50	0
4	DMS	B	8405	4/4	0.97	0.10	38,52,53,63	0
4	DMS	D	8408	4/4	0.97	0.09	23,36,40,100	0
3	NA	D	3101	1/1	0.98	0.03	27,27,27,27	0
2	MG	B	3001	1/1	0.98	0.07	21,21,21,21	0
4	DMS	D	8405	4/4	0.98	0.07	29,31,31,36	0
3	NA	B	3101	1/1	0.98	0.08	29,29,29,29	0
4	DMS	A	8401	4/4	0.98	0.07	14,19,31,33	0
4	DMS	A	8402	4/4	0.98	0.06	14,28,31,58	0
4	DMS	D	8411	4/4	0.98	0.09	26,29,43,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DMS	C	8402	4/4	0.98	0.06	14,28,30,30	0
3	NA	B	3103	1/1	0.98	0.04	25,25,25,25	0
2	MG	B	3002	1/1	0.98	0.05	18,18,18,18	0
4	DMS	C	8405	4/4	0.98	0.07	23,36,39,47	0
3	NA	C	3101	1/1	0.98	0.04	30,30,30,30	0
2	MG	A	3002	1/1	0.98	0.06	23,23,23,23	0
3	NA	A	3101	1/1	0.98	0.06	30,30,30,30	0
4	DMS	B	8401	4/4	0.98	0.05	18,20,29,33	0
4	DMS	B	8402	4/4	0.98	0.06	15,23,29,33	0
4	DMS	D	8701	4/4	0.98	0.10	21,32,32,55	0
4	DMS	D	8401	4/4	0.98	0.05	20,20,27,29	0
4	DMS	D	8402	4/4	0.98	0.07	15,32,33,35	0
2	MG	A	3001	1/1	0.99	0.02	30,30,30,30	0
4	DMS	C	8401	4/4	0.99	0.06	19,21,33,54	0
3	NA	B	3102	1/1	0.99	0.03	19,19,19,19	0
3	NA	D	3102	1/1	0.99	0.02	18,18,18,18	0
2	MG	D	3002	1/1	0.99	0.06	17,17,17,17	0
2	MG	C	3001	1/1	0.99	0.04	20,20,20,20	0
3	NA	A	3103	1/1	0.99	0.03	27,27,27,27	0
4	DMS	D	8412	4/4	0.99	0.07	26,34,45,50	0
3	NA	C	3102	1/1	0.99	0.02	18,18,18,18	0
2	MG	C	3002	1/1	0.99	0.03	17,17,17,17	0
3	NA	A	3102	1/1	1.00	0.03	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.